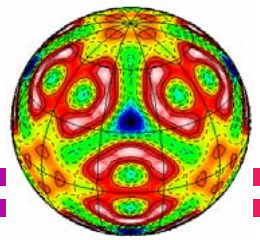

The Flavor of CMSN: What are we about?

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The Mission of the Office of Basic Energy Sciences:

- *Foster and support fundamental research to provide the basis for new, improved, environmentally conscientious energy technologies;*
- *Plan, construct, and operate major scientific user facilities for "materials sciences and related disciplines" to serve researchers from academia, federal laboratories, and industry*

Computational Materials Science Network

The mission of the Computational Materials Science Network is to advance frontiers in computational materials science by assembling diverse sets of researchers committed to working together to solve relevant materials problems that require cooperation across organizational and disciplinary boundaries.

CMSN …

- Is many things according to the eye of the beholder. (But generally positive.)
- Is like the Center of Synthesis and Processing, but it isn't CSP.
  - € It is a theory/computation activity which means there is a greater fraction of the effort assessing what should be done. Since a major theme is spanning length and time scales, one necessary step is to get experts in different length regimes communicating.
  - € CMSN involves many more people from outside the national laboratories. More on that later.
- Shares the spirit of Psi-k, but isn't Psi-k.
  - € CMSN only funds the collaboration costs. There must be base funding for the investigator's research. This is more like CSP and not like Psi-k which has base funding.

Funded Collaborative Research Team Proposals

In FY04, the active teams are:

- Excited State Electronic Structure and Response Functions (J. Rehr & S. Louie)
- Fundamentals of Dirty Interfaces: From Atoms to Alloy Microstructures (A. Karma & A. Rollett)
- Predictive Capability for Strongly Correlated Systems (W. Pickett & R. Scalletar)
- Microscructural Effects on the Mechanics of Materials (R. LeSar & D. Wolf)
- Magnetic Materials Bridging Basic and Applied Science (B. N. Harmon & G.M. Stocks)

Criteria for Cooperative Research Team Proposals

Proposals should:

- focus on critical scientific issue {operationally modified}
- have a clear path to relevance (i.e., real materials issues)
- be of the type best pursued through broad cooperative efforts, as opposed to those key problems best tackled by single investigator groups
- build on existing BES funded programs
- define some short-term deliverables combined with long-term objectives
- a strong synergism with experimental and industrial programs is highly encouraged

And so shall ye be judged!

Evaluating CMSN CRT Proposals

The Standard DMS&E Criteria are

- **Scientific quality**
  - **If it isn't good science, it isn't us.**
  - **A very sizeable fraction of that evaluation occurs for the base program.**
- **Appropriateness of Method**
  - **The "method" of interest for CMSN is first the teaming.**
  - **This does not preclude valuation of any of the methodology.**
- **Adequacy of Personnel and Resources**
- **Reasonableness of Budget**
  - **PLEASE, it is the CMSN addition, not the base program!**
  - **Basically, the budget is fixed. The issue is how well it is used.**

Evaluating CMSN CRT Proposals

-BUT-

The most difficult, and important, additional criterion is that you should evaluate the value of the ***synergism***!

What is being sought is additional value beyond what we would get if we had randomly funded and equal number of workshops, postdocs, students, travel, etc.

CMSN is a Logical Scheme

- Repeating, CMSN funds the coordination costs to pull together a Cooperative Research Team to work on a common project. (Travel, workshops, ***shared*** students and postdocs, and …)
- Logical as it may be, it doesn't fit well DOE bureaucracy!
  - funds to the national laboratories go smoothly but are hard to track √
  - funds to PI with a grant from us can go as a supplement: requires the PI submit a supplement request. √
  - funds to other PI's require some creativity (subcontracts are the most desirable but often entail unacceptable overheads. Writing mini-grants has been strongly discouraged.)